

Correlation between characteristic energies in non- s -wave pairing superconductors

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Abstract

By solution of the Bethe-Goldstone equation for the Cooper pairing problem, an approximate analytic relation is derived between coherence length ξ and the binding energy of the Cooper pair. This relation is then qualitatively confirmed by numerically solving the corresponding self-consistent gap equations, following the crossover from weak to strong coupling, in non- s -wave superconductors. The relation applies to non-conventional superconductors, and in particular to heavy Fermions and to high- T_c cuprates. Utilizing in addition a phenomenological link between $k_B T_c$ and a characteristic energy $\varepsilon_c = \hbar^2/2m^*\xi^2$, with m^* the effective mass, major differences are exposed in the functional relation between $k_B T_c$ and ε_c for s -wave materials and for non-conventional superconductors. The relation between critical temperature and ε_c thereby proposed correctly reflects the qualitative properties of heavy Fermion superconductors.

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1 Introduction

In earlier work [1,2], we have discussed the possible correlation between the critical temperature T_c in anisotropic superconductors and a ‘natural’ energy scale $\varepsilon_c \sim \hbar^2/m^*l_c^2$ involving the effective mass m^* and some characteristic length l_c . Here, by anisotropic superconductors we mean a superconductor characterized by non-spherically symmetric pairing, giving rise to an anisotropic \mathbf{k} -dependence of the gap energy in momentum space. Well-known instances of such materials are the heavy Fermion compounds, most of them being characterized by a p -wave order parameter [3,4], and the high- T_c cuprates, whose order parameter displays d -wave symmetry [5]. The most natural physical choice for the characteristic length l_c entering the definition of ε_c above was the coherence length ξ [1]. In the case of anisotropic superconducting materials in the presence of magnetic fluctuations, we later correlated the coherence length ξ to the spin-fluctuation temperature T_{sf} as $k_{\text{B}}T_{\text{sf}} \sim \hbar^2/m^*\xi^2$ [2].

The possible enhancement of the critical temperature T_c in an anisotropic superconductor was already studied in the early work of Markowitz and Kadanoff [6] within a weak-coupling, BCS-like approach, and more recently revived in Refs. [7,8,9] as possibly relevant for the high- T_c cuprates. A generalization of Markowitz and Kadanoff’s results to the strong and intermediate coupling regime however showed that in the strong coupling limit anisotropy is effectively averaged out, and the gap tends to become isotropic [10].

In the case of the high- T_c cuprates, the strong coupling limit corresponds to the underdoped region of their phase diagram, which is usually interpreted in terms of a crossover between Bose-Einstein condensation of strongly coupled preformed pairs above T_c , and weak coupling, BCS-like superconductivity in the overdoped regime [11]. On the other hand, the coherence length ξ can be continuously connected to the characteristic size of the preformed bosonic pairs in the normal state of (underdoped) high- T_c cuprates. Therefore, the coherence length may serve to parametrize the crossover from weak to strong coupling, with $k_{\text{F}}\xi$ decreasing in going from weak coupling, characterized by large superconducting pair fluctuations, to strong coupling, k_{F} being the Fermi momentum [12] (see also Refs. [13,14], and refs. therein). In the underdoped regime, a relatively short coherence length is consistent with the idea of preformed pairs localized in real space [15,16,17,18]. In such a limit, it is interesting to investigate how the internal structure of these preformed pairs is related to the overall symmetry of the many-body order parameter [19].

Here, we derive an explicit expression for the coherence length in terms of the pair binding energy for the Cooper problem in anisotropic superconductors. Such an expression [see Eq. (13) below] explicitly contains the quantum num-

ber ℓ of the pair relative angular momentum, which is usually employed to parametrize the anisotropic character of the order parameter, $\ell = 0, 1, 2$ corresponding to s -, p -, and d -wave symmetry, respectively. While this expression correctly reduces to the standard one for isotropic s -wave superconductors, in the case $\ell > 0$ it agrees qualitatively with the phenomenological dependence of $k_B T_c$ on the characteristic energy ε_c , proposed in Ref. [1] for the heavy Fermion compounds as well as for the high- T_c cuprates. Such a dependence of the characteristic energy for superconductivity on ε_c is then qualitatively confirmed by numerically solving the self-consistent gap equations for the maximum gap at $T = 0$ in the case of an anisotropic superconductor in the crossover between the weak- and strong-coupling limits, as a function of the dimensionless crossover parameter $k_F \xi$, now employing a more general definition of the coherence length ξ for anisotropic superconductors.

The paper is organized as follows. In Sec. 2, after briefly reviewing the Bethe-Goldstone equation for the Cooper problem in the case of isotropic superconductors, we generalize and solve it for non- s -wave superconductors, characterized by a superconducting instability in the (ℓ, m) channel of relative angular momentum quantum numbers. Our results are discussed in relation to the earlier phenomenological findings in Ref. [1]. In Sec. 3 we analyze the gap equations arising from the corresponding many-body problem at the mean-field level. Although we now have to resort to numerical integration (at least in the non- s -wave case), our results qualitatively confirm the approximate relation between characteristic energies derived in Sec. 2, also in the crossover from weak to strong coupling. In Sec. 4 we eventually summarize and propose some directions for future work.

2 Bethe-Goldstone equation for non- s -wave superconductors

The Bethe-Goldstone equation for the Cooper problem [20] in momentum space reads:

$$(\varepsilon - 2\xi_{\mathbf{k}})\psi_{\mathbf{k}} = \sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'}\psi_{\mathbf{k}'}, \quad (1)$$

where $\psi_{\mathbf{k}}$ is the Fourier transform of the pair wave-function with wave-vector \mathbf{k} (here, we assume a spin-singlet state, with zero total momentum), $\xi_{\mathbf{k}} = \hbar^2 k^2 / (2m^*) - \mu$ is the energy of a single electron with respect to the chemical potential μ , m^* is the effective mass, ε is the binding energy of the electron pair, and $V_{\mathbf{k}\mathbf{k}'}$ is the Fourier transform of the electron-electron interaction (see also Ref. [21] for a pedagogical review). In the weak-coupling limit, we may safely assume $\mu = \varepsilon_F$ at $T = 0$, with ε_F the Fermi energy. However, we anticipate that this identification will be superseded in Sec. 3, where the crossover from weak to strong coupling will be addressed more in detail. In the case of anisotropic superconductors, we adopt the spirit of the Anderson-

Brinkman-Morel model for p -wave superfluidity in ^3He [22], and expand the electron-electron interaction in spherical harmonics around the Fermi surface as

$$V_{\mathbf{k}\mathbf{k}'} = -\frac{1}{\Omega} \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} V_{\ell m} Y_{\ell m}(\hat{\mathbf{k}}) Y_{\ell m}(\hat{\mathbf{k}}'), \quad (2)$$

for $|\xi_{\mathbf{k}}|, |\xi_{\mathbf{k}'}| < \Lambda$, and zero otherwise, where $\hat{\mathbf{k}}$ is the unit vector pointing along the direction of \mathbf{k} , Ω denotes the volume of the system, and Λ is an energy cut-off, characterized by the nature of the interaction. In the case of conventional superconductivity (s -wave pairing, or $\ell = 0$), it would be natural to identify such an energy scale with the Debye energy, as in BCS theory.

The use of spherical harmonics to expand the electron-electron interaction in anisotropic pairing superconductors characterized by a spherical Fermi surface was earlier considered by Markowitz and Kadanoff [6] in the weak-coupling regime (see also Refs. [8,9]), and later by Combescot [10] in the strong and intermediate coupling regime. A related model of exotic Cooper pairing with finite angular momentum has been discussed also in Ref. [23], where rotational symmetry breaking ($\ell > 0$) is due to the interplay between the finite range of the attractive potential and the interelectronic average distance. Within such model, the authors of Ref. [23] also derive the ℓ -dependence of the critical temperature in the Bose-Einstein limit. In the more realistic case of a non-spherical Fermi surface, spherical harmonics are naturally replaced by Allen's Fermi surface harmonics [24], which have been used by Whitmore *et al.* [7] in extending the results of Ref. [6] within the framework of Eliashberg equations for T_c . Moreover, spherical harmonics afford a natural classification of anisotropic superconductors (such as heavy Fermion compounds [3,4] as well as high- T_c cuprates [5]) in terms of their pairing symmetry.

Within the weak-coupling approximation, the largest attractive coupling constant $V_{\ell m} \equiv V > 0$ in Eq. (2) gives rise to a pairing instability in the (ℓ, m) channel. In the following, we shall neglect other instabilities, which may arise well below T_c , corresponding to mixed symmetry pairing. This amounts to retaining the (ℓ, m) term only in the expansion Eq. (2). In this case, Eq. (1) has a solution given by

$$\psi_{\mathbf{k}} = \alpha \frac{Y_{\ell m}(\hat{\mathbf{k}})}{\varepsilon - 2\xi_{\mathbf{k}}} \quad (3)$$

belonging to the eigenvalue

$$\varepsilon \simeq -2\Lambda \exp\left(-\frac{2}{VN(0)}\right), \quad (4)$$

where $N(0)$ is the density of states at the Fermi level, and α is a normalization constant. Such a solution corresponds to a bound state ($\varepsilon < 0$), and a further mean-field analysis of the many-electron problem (see also Sec. 3) shows that it indeed corresponds to a superconducting state, characterized by a gap function

at $T = 0$:

$$\Delta_{\hat{\mathbf{k}}} = 2\Lambda\Gamma e^{-1/N(0)V} Y_{\ell m}(\hat{\mathbf{k}}), \quad (5)$$

having the symmetry of the attractive channel under consideration, where:

$$\ln \Gamma = - \int d\Omega_{\mathbf{k}} |Y_{\ell m}(\hat{\mathbf{k}})|^2 \ln |Y_{\ell m}(\hat{\mathbf{k}})|, \quad (6)$$

the integration being carried over the unit sphere [25]. The anisotropic \mathbf{k} -dependence of the pair wave-function $\psi_{\mathbf{k}}$ in Eq. (3) in the case $\ell > 0$ provides interesting information on the internal structure of a Cooper pair and its connection with the overall symmetry of the many-body gap function.

Given the pair wave-function $\psi_{\mathbf{k}}$, the coherence length ξ is naturally defined by

$$\xi^2 = \frac{\sum_{\mathbf{k}} |\nabla_{\mathbf{k}} \psi_{\mathbf{k}}|^2}{\sum_{\mathbf{k}} |\psi_{\mathbf{k}}|^2}. \quad (7)$$

Passing to the continuous limit, in the isotropic, s -wave case ($\ell = 0$), one obtains [21]

$$\xi^2 = \frac{2\hbar^2}{3m^*\varepsilon_F} \frac{1}{x^2}, \quad (8)$$

where $x = |\varepsilon|/(2\varepsilon_F)$ measures the binding energy of a pair in units of the energy of an unbound pair. Apart from a numerical factor, from Eq. (8) one thus recovers the correct order of magnitude relation between the critical temperature, the Fermi velocity $v_F = \hbar^{-1} d\xi_{\mathbf{k}}/dk$, and the coherence length:

$$k_B T_c \sim |\varepsilon| \sim \frac{\hbar v_F}{\xi}. \quad (9)$$

In the anisotropic case, for a pairing instability in the (ℓ, m) channel, with the pair wave-function given by Eq. (3), the denominator in Eq. (7) is easily integrated in the continuous limit as

$$\begin{aligned} \sum_{\mathbf{k}} |\psi_{\mathbf{k}}|^2 &\rightarrow \Omega \int d^3\mathbf{k} |\psi_{\mathbf{k}}|^2 \\ &= \frac{\Omega\alpha^2}{4\pi} \int_0^\infty dE \frac{N(E)}{(\varepsilon - 2E)^2} \int d\Omega_{\mathbf{k}} |Y_{\ell m}(\hat{\mathbf{k}})|^2 \\ &\approx -\Omega\alpha^2 \frac{N(0)}{8\pi\varepsilon}, \end{aligned} \quad (10)$$

where $N(E)/4\pi$ is the density of states per unit solid angle, and use has been made of the normalization condition of the spherical harmonics. In the case $\ell \neq 0$, the anisotropic \mathbf{k} dependence of the pair wave-function Eq. (3) gives rise to two contributions in the numerator of Eq. (7), according to the chain

rule

$$|\nabla_{\mathbf{k}}\psi_{\mathbf{k}}|^2 = \frac{\alpha^2}{k^2} \frac{|\nabla_{\hat{\mathbf{k}}}Y_{\ell m}(\hat{\mathbf{k}})|^2}{(\varepsilon - 2\xi_{\mathbf{k}})^2} + 4\alpha^2\hbar^2v_F^2 \frac{|Y_{\ell m}(\hat{\mathbf{k}})|^2}{(\varepsilon - 2\xi_{\mathbf{k}})^4}. \quad (11)$$

Here, we have made use of the decomposition $\nabla_{\mathbf{k}} = k^{-1}\nabla_{\hat{\mathbf{k}}} + \hat{\mathbf{k}}\partial/\partial k$, where $\nabla_{\hat{\mathbf{k}}}$ denotes the angular part of the gradient operator in momentum space, and of the fact that $\xi_{\mathbf{k}}$ depends only on $k = |\mathbf{k}|$. Passing to the continuous limit, integrating separately over the angles as in Eq. (10), and making use of the identity

$$\begin{aligned} \int d\Omega_{\mathbf{k}} |\nabla_{\hat{\mathbf{k}}}Y_{\ell m}(\hat{\mathbf{k}})|^2 &= - \int d\Omega_{\mathbf{k}} Y_{\ell m}^*(\hat{\mathbf{k}}) \nabla_{\hat{\mathbf{k}}}^2 Y_{\ell m}(\hat{\mathbf{k}}) \\ &= \ell(\ell + 1), \end{aligned} \quad (12)$$

which follows from a variant of the Green's formula over the unit sphere, one eventually obtains

$$\xi^2 = \frac{\hbar^2}{2m^*\varepsilon_F} \left[\frac{4}{3} \frac{1}{x^2} + \frac{\ell(\ell + 1)}{1 + x} \left(1 - \frac{x \ln x}{1 + x} \right) \right]. \quad (13)$$

Equation (13) implicitly relates the binding energy $|\varepsilon|$ of a Cooper pair to its characteristic size ξ for anisotropic pairing superconductors.

In the case of non- s -wave superconductors, Equation (13) manifestly includes an ‘orbital’ contribution, proportional to $\ell(\ell + 1)$, as earlier surmised in Ref. [1] on the basis of phenomenological considerations. There, we proposed the existence of a phenomenological relation linking $k_B T_c$ to the characteristic energy

$$\varepsilon_c = \frac{\hbar^2}{2m^*\xi^2}, \quad (14)$$

in the case of anisotropic superconductors. That the effective mass m^* should enter inversely in determining the scale of $k_B T_c$ was earlier recognized by Uemura *et al.* [26], who did not, however, include the coherence length in their analysis [12]. By comparing the experimental values for several heavy Fermion compounds (p -wave superconductors, $\ell = 1$) as well as high- T_c superconductors (d -wave superconductors, $\ell = 2$), in the anisotropic case we found that $k_B T_c = f(\varepsilon_c)$ deviates from the square-root behavior, $k_B T_c \propto \sqrt{\varepsilon_c}$, that is easily derived from Eqs. (9) and (14) for isotropic, s -wave superconductors. In particular, in the heavy Fermion case, we noticed a large initial slope in $f(\varepsilon_c)$ for $\varepsilon_c = 0$, and a tendency of such function to approach saturation, as ε_c increases.

In view of the fact that $k_B T_c \sim |\varepsilon| \sim x\varepsilon_F$ [21], Eq. (13) implicitly defines the generalization to the anisotropic case of the relationship between $k_B T_c$ and ε_c we were looking for. Equation (13) correctly reduces to Eq. (8) in

the isotropic case (s -wave superconductors, $\ell = 0$). In the case of non- s -wave superconductors ($\ell > 0$), Eq. (13) indeed increases with increasing ε_c , starting with a logarithmically infinite slope at $\varepsilon_c = 0$, and tending to a saturation value as $\varepsilon_c \rightarrow \infty$. Such a limit is *e.g.* approached for $k_F \xi \ll 1$. Setting $a = 4/[3\ell(\ell + 1)]$ and performing an asymptotic analysis of Eq. (13), in the limit $k_F \xi \ll 1$ ($\ell > 0$) one obtains

$$x = \frac{1 + a}{W[(1 + a)/e]}, \quad (15)$$

where $W(z)$ is Lambert's function [27], and in the limit of very large anisotropy ($\ell \gg 1$):

$$\lim_{\ell \rightarrow \infty} x = W^{-1}(e^{-1}) = 3.591 \dots \quad (16)$$

Figure 1 shows the dependence of the dimensionless measure of the pair binding energy $x = |\varepsilon|/2\varepsilon_F$ on $\varepsilon_c/\varepsilon_F = (k_F \xi)^{-2}$, implicitly defined by Eq. (13) in the cases $\ell = 0, 1, 2$, corresponding to s -, p -, and d -wave superconductivity, respectively. Keeping fixed all other variables, one notices that for $\xi > \xi_0$, where

$$\frac{\hbar^2}{2m^* \xi_0^2 \varepsilon_F} = \frac{3}{4W^2(e^{-1})} = 9.672 \dots, \quad (17)$$

$|\varepsilon|$ increases as ℓ increases while, for $\xi < \xi_0$, $|\varepsilon|$ decreases as ℓ increases, although without large deviations from the limiting value, Eq. (16). Therefore, at least for sufficiently weakly coupled superconductors ($\xi > \xi_0$), anisotropy enhances superconductivity, the degree of anisotropy being here parametrized by the order ℓ of the spherical harmonic modelling the \mathbf{k} dependence of the order parameter.

3 Mean-field analysis of the many-body problem and the crossover from weak to strong coupling

The definition of the Cooper pair size ξ we employ in Eq. (7) makes use of the pair wave-function $\psi_{\mathbf{k}}$ for the Cooper problem, in which the only many-body effect is that of forbidding the occupancy of states below the Fermi level, ε_F . Within BCS theory, *i.e.* at the mean field level, a self-consistent treatment of the superconducting instability affords a better definition of the pair wave-function, which in momentum space is given by [21] $\psi_{\mathbf{k}} = \Delta_{\mathbf{k}}/(2E_{\mathbf{k}})$, where $\Delta_{\mathbf{k}}$ is the gap function, now depending on \mathbf{k} as a vector, and $E_{\mathbf{k}} = (\xi_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2)^{1/2}$ the upper branch of the quasiparticle dispersion relation. With this definition of $\psi_{\mathbf{k}}$, when $E_{\mathbf{k}}$ is allowed to vanish locally on the Fermi surface, as is the case for p - and d -wave superconductors, it has been recently shown that nodal quasiparticles give rise to a logarithmically divergent contribution to ξ , as defined by Eq. (7) [28]. While such a drawback does not arise in s -wave superconductors [29], in the case of anisotropic superconductors the

coherence length must be defined in terms of the range in real space of the static correlation function for the modulus of the order parameter [30,28]. The fact that our result Eq. (13) provides a finite estimate for ξ also in the anisotropic case clearly depends on our approximate choice for $\psi_{\mathbf{k}}$, which solves only the two-body Cooper problem.

In order to discuss the limits of validity of the approximate results derived in Sec. 2, we will then work out numerically the mean-field solution to the corresponding BCS Hamiltonian, both in the weak and in the strong-coupling limit. We start by reviewing the model and notations set out in Refs. [12,30,29,28] (see also Ref. [31]).

We shall consider the following Hamiltonian for a superconducting system in three dimensions [32]:

$$H = \sum_{\mathbf{k}\sigma} \xi_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}} V_{\mathbf{k}\mathbf{k}'} c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}+\mathbf{q}\downarrow}^\dagger c_{-\mathbf{k}'+\mathbf{q}\downarrow} c_{\mathbf{k}'\uparrow}, \quad (18)$$

where $c_{\mathbf{k}\sigma}^\dagger$ [$c_{\mathbf{k}\sigma}$] is the creation [destruction] operator for an electron with wave-vector \mathbf{k} and spin projection $\sigma \in \{\uparrow, \downarrow\}$ along a specified direction, $\xi_{\mathbf{k}} = \hbar^2 k^2 / (2m^*) - \mu$ is the dispersion relation for free electrons with effective mass m^* , measured with respect to the chemical potential μ , and

$$V_{\mathbf{k}\mathbf{k}'} = -\frac{V}{\Omega} Y_{\ell m}(\hat{\mathbf{k}}) Y_{\ell m}(\hat{\mathbf{k}}') \quad (19)$$

is the projection of the electron-electron interaction along the (ℓ, m) channel, as in Eq. (2), which we assume to be attractive ($V > 0$) [33]. Equation (19) generalizes to the non- s -wave case the contact potential in real space discussed *e.g.* by Marini *et al.* [29]. Standard diagonalization techniques then lead to the mean-field coupled equations for the gap energy $\Delta_{\mathbf{k}} = \Delta_0 Y_{\ell m}(\hat{\mathbf{k}})$ and the particle density n at $T = 0$ (see Ref. [31] for the case $T \neq 0$):

$$\frac{1}{V} = \frac{1}{\Omega} \sum_{\mathbf{k}} \frac{|Y_{\ell m}(\hat{\mathbf{k}})|^2}{2E_{\mathbf{k}}}, \quad (20a)$$

$$n = \frac{2}{\Omega} \sum_{\mathbf{k}} v_{\mathbf{k}}^2, \quad (20b)$$

where $v_{\mathbf{k}}^2 = \frac{1}{2}(1 - \xi_{\mathbf{k}}/E_{\mathbf{k}})$, together with $u_{\mathbf{k}}^2 = 1 - v_{\mathbf{k}}^2$, are the usual coherence factors of BCS theory.

Owing to our choice of a free particle dispersion relation (all band effects are embedded in a single parameter, namely the effective mass m^*), and of a contact potential in real space, the sums over \mathbf{k} in Eq. (20a) above give rise to an ultraviolet divergence, which requires a suitable regularization. In three

dimensions, it is customary to introduce the scattering amplitude a_s [30,29,34], which for our anisotropic interaction reads:

$$\frac{m^*}{4\pi a_s} = -\frac{1}{V} + \frac{1}{\Omega} \sum_{\mathbf{k}} \frac{m^*}{k^2} |Y_{\ell m}(\hat{\mathbf{k}})|^2. \quad (21)$$

Subtracting Eq. (21) from Eq. (20a) one has:

$$-\frac{m^*}{4\pi a_s} = \frac{1}{\Omega} \sum_{\mathbf{k}} \left(\frac{1}{2E_{\mathbf{k}}} - \frac{m^*}{k^2} \right) |Y_{\ell m}(\hat{\mathbf{k}})|^2. \quad (22)$$

Following Ref. [29], we render Eqs. (20) and Eq. (22) dimensionless, by introducing the dimensionless quantities

$$x^2 = \frac{\hbar^2 k^2}{2m^* \Delta_0}, \quad x_0 = \frac{\mu}{\Delta_0},$$

$$\xi_x = \frac{\xi_{\mathbf{k}}}{\Delta_0} = x^2 - x_0, \quad E_x = \frac{E_{\mathbf{k}}}{\Delta_0} = \sqrt{\xi_x^2 + |Y_{\ell m}(\hat{\mathbf{x}})|^2},$$

and the Fermi energy $\varepsilon_F = \hbar^2 k_F^2 / (2m^*) = \hbar^2 (3\pi^2 n)^{2/3} / (2m^*)$. In particular, Marini *et al.* [29] observe that $x_0 = \mu / \Delta_0$ can be used as a parameter for the crossover between the strong-coupling, Bose-Einstein (BE) limit ($x_0 \ll 0$) and the weak-coupling, BCS limit ($x_0 \gg 0$). Moreover, on one hand, the expression resulting from the dimensionless version of Eq. (22) for $(k_F a_s)^{-1}$ can be inverted to obtain x_0 as a function of the dimensionless scattering length $k_F a_s$. On the other hand, one may alternatively use $k_F \xi$ as the independent variable in place of $k_F a_s$ [29]. Indeed, it was earlier recognized by Pistoiesi and Strinati [12] (following the seminal work of Nozières and Schmitt-Rink [15]) that a natural variable which can be used to follow the crossover from strong-coupling to weak-coupling superconductivity is the product $k_F \xi$ of Fermi wave-vector k_F times the coherence length ξ for two-electron correlation. In the BE limit, electrons are expected to bind in quasi-bound pairs localized in real space (Schafroth pairs [35]), thus realizing the condition $k_F \xi \ll 1$, while the BCS limit corresponds to loosely coupled pairs, with $k_F \xi \gg 1$, localized in momentum space close to the Fermi energy.

A zero-temperature calculation of the coherence length for a three-dimensional, s -wave superconductor along the crossover between the weak- and the strong-coupling limits has been performed both numerically [30] and analitically [29]. The case of a two-dimensional, d -wave superconductor has been discussed in Ref. [28], where a dispersion relation typical of the cuprate superconductors has been explicitly considered. As anticipated above, in the non- s -wave case ($\ell \neq 0$), the standard definition, Eq. (7), of the coherence length leads to unphysical divergences. One may still conveniently define a coherence length as the range in real space of the static correlation function $X_{\Delta}(\mathbf{r})$ for the modulus

of the order parameter [30,28] as

$$\xi^{-1} = - \lim_{r \rightarrow \infty} \frac{\log X_{\Delta}(r)}{r}. \quad (23)$$

The Fourier transform $X_{\Delta}(\mathbf{q})$ of such a function has been derived for an s - and a d -wave superconductor in Refs. [30] and [28], respectively. In the case of our anisotropic interaction, Eq. (19), it reads:

$$\begin{aligned} X_{\Delta}(\mathbf{q})^{-1} &= \frac{1}{V} - \frac{1}{2\Omega} \sum_{\mathbf{k}} |Y_{\ell m}(\hat{\mathbf{k}})|^2 \frac{(u_{\mathbf{k}+\mathbf{q}/2} u_{\mathbf{k}-\mathbf{q}/2} - v_{\mathbf{k}+\mathbf{q}/2} v_{\mathbf{k}-\mathbf{q}/2})^2}{E_{\mathbf{k}+\mathbf{q}/2} + E_{\mathbf{k}-\mathbf{q}/2}} \\ &= \frac{1}{2\Omega} \sum_{\mathbf{k}} |Y|^2 \left[\frac{1}{E} - \frac{1}{E_+ + E_-} \left(1 + \frac{\xi_+ \xi_- - |\Delta_+| |\Delta_-|}{E_+ E_-} \right) \right], \end{aligned} \quad (24)$$

where $E \equiv E_{\mathbf{k}}$, $Y \equiv Y_{\ell m}(\hat{\mathbf{k}})$, ξ_{\pm} , Δ_{\pm} , E_{\pm} are calculated at momenta $\mathbf{k} \pm \mathbf{q}/2$, respectively, and use has been made of the gap equation, Eq. (20a), in going into the second line.

First of all, since the summand in Eq. (24) depends only on $k = |\mathbf{k}|$, $q = |\mathbf{q}|$, and on the relative angle between \mathbf{k} and \mathbf{q} , passing to the continuum limit and transforming the sums over wave-vectors into an integral, one has $X_{\Delta}(\mathbf{q}) \equiv X_{\Delta}(q)$. Moreover, $X_{\Delta}(q)$ is an even function of its argument. Back to real space, one analogously has $X_{\Delta}(\mathbf{r}) \equiv X_{\Delta}(r)$. Then, the asymptotic behaviour of $X_{\Delta}(r)$ at large distance r will be governed by the behaviour of its Fourier transform $X_{\Delta}(q)$ at small wave-vector q . In particular, assuming the expansion [30,28]:

$$X_{\Delta}^{-1}(q) = a + bq^2 + O(q^4), \quad (25)$$

it is straightfoward to show [30] that

$$\xi^2 = \frac{b}{a}. \quad (26)$$

Such a definition of the coherence length is now consistent also for nodal superconductors [28]. It reduces to Eq. (7) in the weak-coupling limit for the s -wave case, and applies also to the strong-coupling regime, provided $b > 0$ (given that $a > 0$, identically, provided $\Delta_0 \neq 0$), *i.e.* provided that $X_{\Delta}(q)$ has its absolute minimum at $q = 0$ [36].

We have numerically solved the gap equations, Eqs. (20), and evaluated the dimensionless coherence length $k_F \xi$ according to this more general definition, Eq. (26), for the anisotropic potential Eq. (19), with $\ell = 0, 1, 2$, corresponding to s -, p -, and d -wave pairing, respectively. Here, a convenient measure of the characteristic energy for superconductivity may be taken as the maximum gap Δ_{\max} , where $\Delta_{\max} \propto k_B T_c$ holds also for anisotropic superconductors [10]. Such a quantity is readily extracted from the solution of the gap equations, Eqs. (20). In Figure 2, we plot the dimensionless characteristic energy

$2\Delta_{\max}/\varepsilon_F$ versus $\varepsilon_c/\varepsilon_F = (k_F\xi)^{-2}$ in the cases $\ell = 0, 1, 2$. As $k_F\xi$ decreases [$(k_F\xi)^{-2}$ increases], one crosses over from the weak-coupling, BCS limit into the strong-coupling, BE limit [12]. Despite a mean-field solution of the self-consistent gap equations has been now taken into account in the calculation, and a more general and consistent definition of the coherence length has been employed, our numerical results are in good qualitative agreement with the approximate results of Sec. 2, with $2\Delta_{\max}/\varepsilon_F$ increasing as a function of $\varepsilon_c/\varepsilon_F$ with a steeper slope, as ℓ increases from $\ell = 0$ (*s*-wave) to $\ell = 2$ (*d*-wave), all curves tending to saturation, at least within the numerically accessible range of the crossover parameter $k_F\xi$. These results are in agreement with the phenomenological plots correlating characteristic energies for both the heavy Fermion and cuprate superconductors in Refs. [1,2].

4 Summary and future directions

We have studied the Cooper problem for an anisotropic superconductor characterized by an electron-electron interaction expanded in terms of simple spherical harmonics over the Fermi sphere. In the weak-coupling limit of a superconducting instability in the (ℓ, m) channel, we have derived an analytical expression for the relation between the pair binding energy and the correlation length, for arbitrary relative angular momentum quantum number ℓ . While such an expression correctly reduces to the standard one in the *s*-wave case ($\ell = 0$), in view of the fact that $k_B T_c$ scales with such a pair binding energy, in the case of non-*s*-wave superconductors ($\ell > 0$) our expression agrees qualitatively with the phenomenological correlation between $k_B T_c$ and the characteristic energy $\hbar^2/(2m^*\xi^2)$ earlier found in Ref. [1]. These results have been confirmed by a numerical solution of the self-consistent gap equations in the crossover between the weak- and the strong-coupling limits, where a more general definition for the coherence length has been employed, applying to anisotropic superconductors.

It may, in the future, prove of significance to include the effect of Coulomb interaction on the formation of Cooper pairs in superconducting assemblies along lines such as those laid down in Ref. [37] (see also Ref. [38]). The question arises then as to whether, in the future, it will be of significance in making the present study the basis of fully quantitative calculations, to generalize beyond the result here, and of course, of many earlier workers, that the Cooper pairs formed as a consequence of an attractive interaction correspond to a single value of the binding energy at a given temperature. There is some evidence (see, *e.g.*, Refs. [39,40]) that some physical properties, and in particular specific heat and tunneling spectra of cuprate materials, may require generalization to Cooper pairs with a finite range of binding energies. We do not anticipate that the qualitative trends proposed in the present paper will be grossly affected.

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- [33] Within this model, the effect of a repulsive Coulomb interaction can be included as an on-site repulsive Hubbard term, so that the interaction potential, Eq. (19), would read $\Omega V_{\mathbf{k}\mathbf{k}'} = U - V Y_{\ell m}(\hat{\mathbf{k}}) Y_{\ell m}(\hat{\mathbf{k}}')$, with $U > 0$. The character of such a contribution would then be *s*-wave, and for a separable choice of the interaction potential it would then affect other *s*-wave components only. Indeed, by numerically solving the self-consistent gap equations for a separable potential allowing for mixed symmetry, some of the present authors have shown that a repulsive onsite $U > 0$ would reduce the mean-field solution for T_c associated to a superconducting instability in the *s*-wave channel, while leaving an instability in other, orthogonal channels unaffected [41]. In the present case, since we are interested only in the superconducting instability in one symmetry channel at a time, the effect of a nonzero (positive) U would then only affect the $\ell = 0$ case, by a simple renormalization of the coupling constant ($-V_{00}/4\pi \mapsto U - V_{00}/4\pi$).
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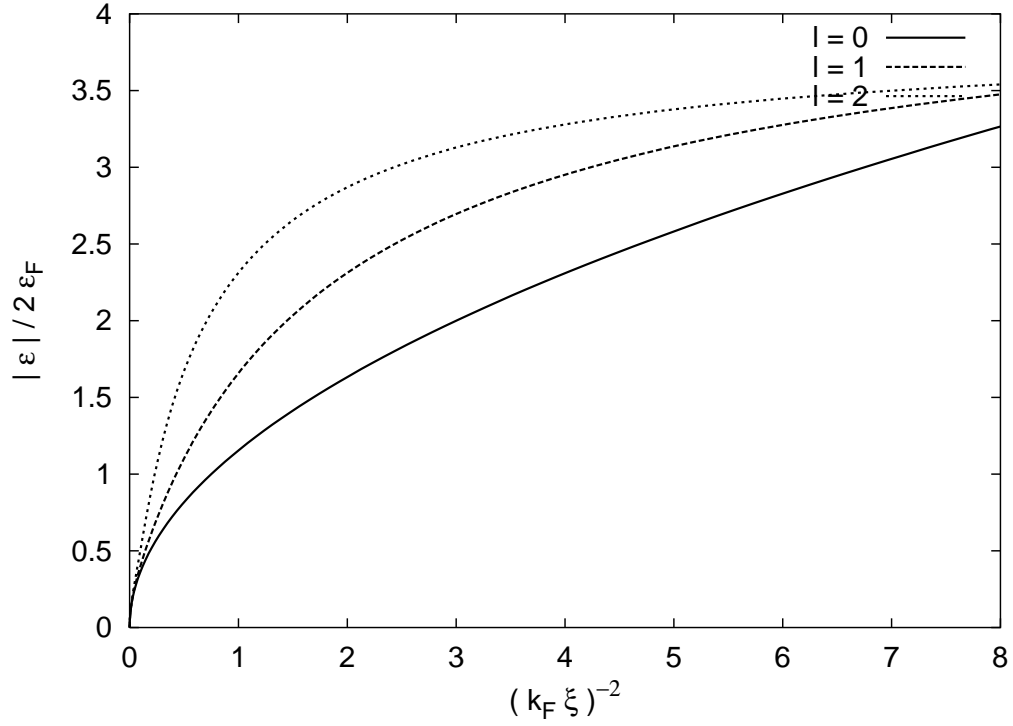


Fig. 1. Dependence of the normalized Cooper pair binding energy $|\epsilon|/2\epsilon_F$ on the characteristic energy $\epsilon_c/\epsilon_F = [\hbar^2/(2m^*\xi^2)]/\epsilon_F = (k_F\xi)^{-2}$, as implicitly defined by Eq. (13), for $\ell = 0, 1, 2$, corresponding to s -, p -, and d -wave superconductivity, respectively. See text for discussion.

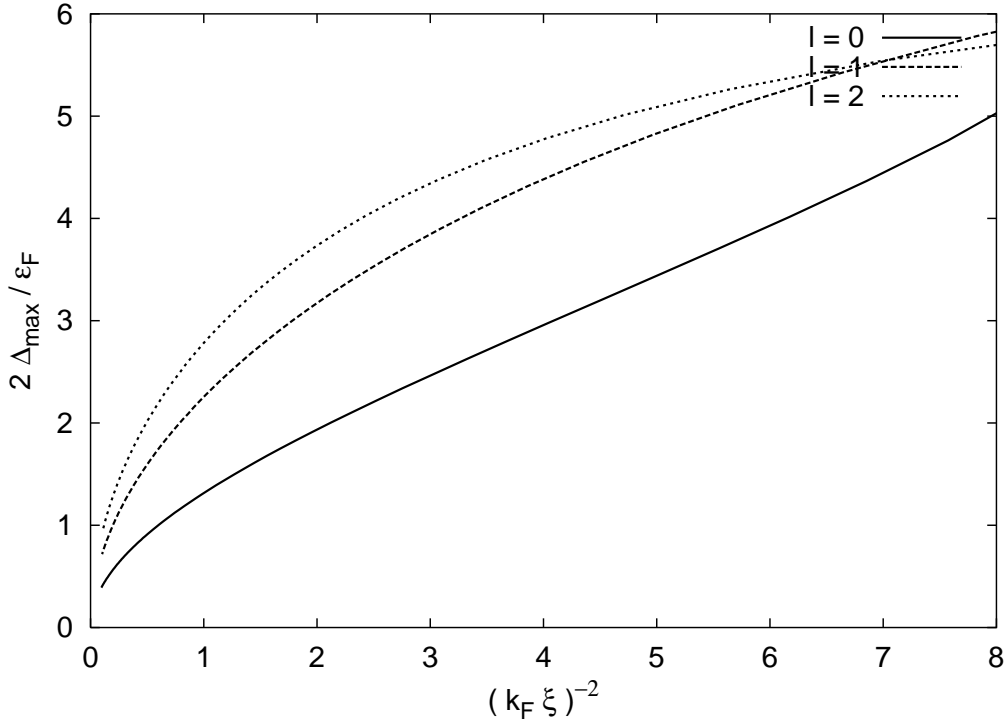


Fig. 2. Dependence of twice the normalized maximum gap energy $2\Delta_{\max}/\varepsilon_F$ on the characteristic energy $\varepsilon_c/\varepsilon_F = (k_F\xi)^{-2}$, for $\ell = 0, 1, 2$, corresponding to s -, p -, and d -wave superconductivity, respectively. As $k_F\xi$ decreases [*i.e.*, $(k_F\xi)^{-2}$ increases] one crosses over from the weak-coupling, BCS limit, to the strong-coupling, BE limit.